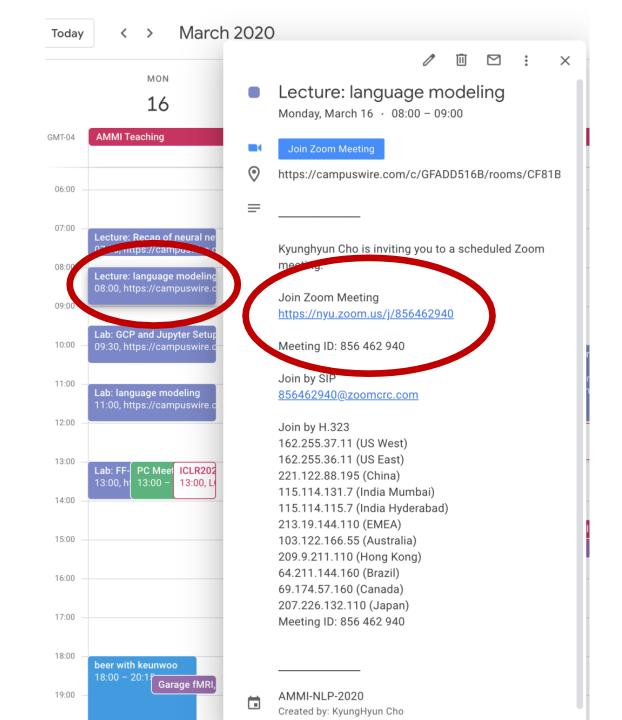
### Zoom meeting ID

- Calendar URL:
   <a href="https://bit.ly/3aYQRkg">https://bit.ly/3aYQRkg</a>
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#### Course discussion/Q&A

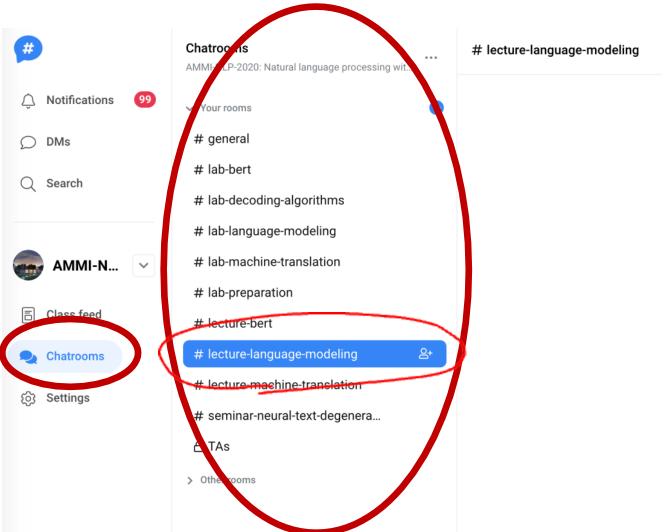
• URL:

https://campuswire.com/p/GFADD516B

• Code: 9109

• Please join now!

• Q&A using chatrooms



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# Recap: Supervised Machine Learning

You all know already, but it's important enough to warrant repetition.

### Supervised Learning - Overview

#### • Provided:

- 1. a set of N input-output "training" examples  $D = \{(x_1, y_1), \dots, (x_N, y_N)\}$
- 2. A per-example loss function  $l(M(x), y) \ge 0$
- 3. Evaluation sets\*: validation and test examples  $D_{\text{val}}$   $D_{\text{test}}$

#### • What we must decide:

- 1. Hypothesis sets  $\mathcal{H}_1, \ldots, \mathcal{H}_M$ 
  - Each set consists of all compatible models
- 2. Optimization algorithm

Often it is necessary to design a loss function.

\* Often these sets are created by holding out subsets of training examples.

### Supervised Learning – Overview

- Given:
  - 1.  $(D \neq \{(x_1, y_1), \dots, (x_N, y_N)\}\)$  and  $D_{\text{val}}, D_{\text{test}}$
  - 2.  $l(M(x), y) \ge 0$
  - 3.  $\mathcal{H}_1,\ldots,\mathcal{H}_M$
  - 4. Optimization algorithm
- Supervised learning finds an appropriate algorithm/model automatically
  - 1. For each hypothesis set  $\mathcal{H}_m$ , find the best model:

$$\hat{M}_m = \arg\min_{M \in \mathcal{H}_m} \sum_{n=1}^{N} l(M(x_n), y_n)$$

using the optimization algorithm.

### Supervised Learning – Overview

- Given:
  - 1.  $D = \{(x_1, y_1), \dots, (x_N, y_N)\}\$ and  $D_{\text{val}}, D_{\text{test}}$
  - 2.  $l(M(x), y) \ge 0$
  - 3.  $\mathcal{H}_1,\ldots,\mathcal{H}_M$
  - 4. Optimization algorithm
- Supervised learning finds an appropriate algorithm/model automatically
  - 1. [Training] For each hypothesis set  $\mathcal{H}_m$ , find the best model:

$$\hat{M}_m = \arg\min_{M \in \mathcal{H}_m} \sum_{n=1}^{\infty} l(M(x_n), y_n)$$

using the optimization algorithm and the training set.

### Supervised Learning - Overview

- Given:
  - 1.  $D = \{(x_1, y_1), \dots, (x_N, y_N)\}\$ and  $D_{\text{val}}, D_{\text{test}}$
  - 2.  $l(M(x), y) \ge 0$
  - 3.  $\mathcal{H}_1,\ldots,\mathcal{H}_M$
  - 4. Optimization algorithm
- Supervised learning finds an appropriate algorithm/model automatically
  - 2. [Model Selection]\* Among the trained models, select the best one

$$\hat{M} = \arg\min_{M \in \{\mathcal{H}_1, \dots, \mathcal{H}_M\}} \sum_{(x,y) \in D_{\text{val}}} l(M(x), y)$$
 using the **validation set** loss.

<sup>\*</sup> If you're familiar with deep learning, "hyperparameter optimization" may be a more familiar term for you.

### Supervised Learning - Overview

- Given:
  - 1.  $D = \{(x_1, y_1), \dots, (x_N, y_N)\}\$ and  $D_{\text{val}}, D_{\text{test}}$
  - 2.  $l(M(x), y) \ge 0$
  - 3.  $\mathcal{H}_1,\ldots,\mathcal{H}_M$
  - 4. Optimization algorithm
- Supervised learning finds an appropriate algorithm/model automatically
  - 3. [Reporting] Report how well the best model would work

$$R(\hat{M}) \approx \frac{1}{|D_{\rm test}|} \sum_{(x,y) \in D_{\rm test}} l(\hat{M}(x),y)$$
 using the test set loss.

<sup>\*</sup> If you're familiar with deep learning, "hyperparameter optimization" may be a more familiar term for you.

### Supervised Learning – Overview

#### • Given:

- 1.  $D = \{(x_1, y_1), \dots, (x_N, y_N)\}\$ and  $D_{\text{val}}, D_{\text{test}}$
- 2.  $l(M(x), y) \ge 0$
- 3.  $\mathcal{H}_1,\ldots,\mathcal{H}_M$
- 4. Optimization algorithm
- Supervised learning finds an appropriate algorithm/model automatically
- It results in an algorithm  $\hat{M}$  with an expected performance of  $R(\hat{M})$

### Supervised Learning

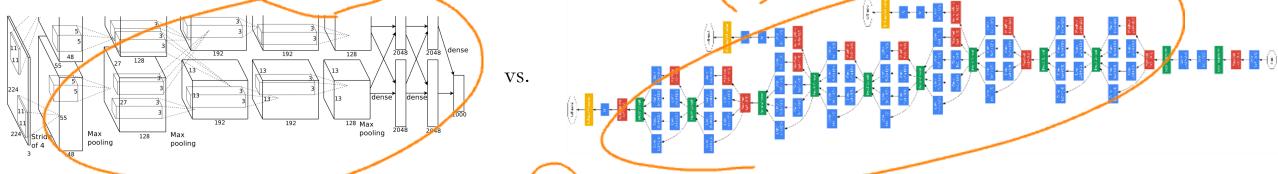
- Three points to consider both in research and in practice
  - 1. How do we decide/design a hypothesis set?
  - 2. How do we decide a **loss function**?
  - 3. How do we **optimize** the loss function?

#### Hypothesis set – Neural Networks

- What kind of machine learning approach will we consider?
  - Classification:
    - Support vector machines, Naïve Bayes classifier, logistic regression, ...?
  - Regression:
    - Support vector regression, Linear regression, Gaussian process, ...?
- How are the hyperparameters sets?
  - Support vector machines: regularization coefficient (C)
  - Gaussian process: kernel function  $k(\cdot, \cdot)$

### Hypothesis set – Neural Networks

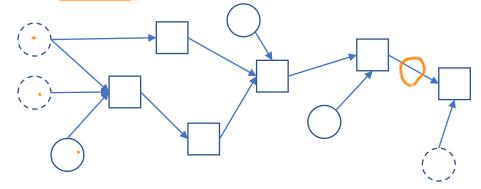
- In the case of deep learning/artificial neural networks,
  - 1. The architecture of a network defines a set  $\mathcal{H}$



- 2. Each model in the set  $M \in \mathcal{H}$  is characterized by its parameters  $\theta$ 
  - Weights and bias vectors define one model in the hypothesis set.
- There are infinitely many models in a hypothesis set.
- We use optimization to find "a" good model from the hypothesis set.

#### Network Architectures

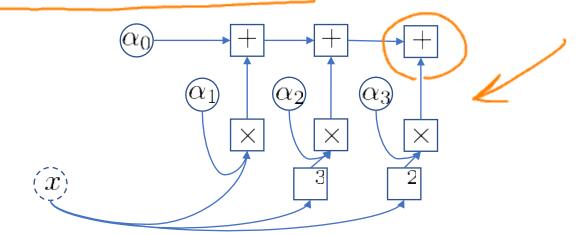
• What is a neural network? – An (arbitrary) directed acyclid graph (DAG)



- 1. Solid Circles parameters (to be estimated or found)
- 2. Dashed Circles vector inputs/outputs (given as a training example)
- 3. Squares compute nodes (functions, often continuous/differentiable)

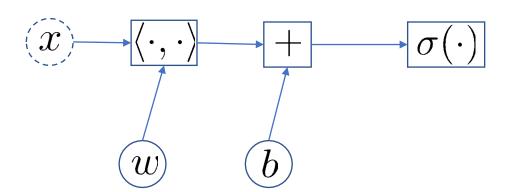
#### Network Architectures

- What is a neural network? An (arbitrary) directed acyclic graph (DAG)
  - 1. Logistic regression  $p_{\theta}(y=1|x) = \sigma(w^{\top}x+b) = \frac{1}{1+\exp(-w^{\top}x-b)}$
  - 2. 3<sup>rd</sup>-order polynomial function  $y = \alpha_0 + \alpha_1 x + \alpha_2 x^2 + \alpha_3 x^3$



#### Inference – Forward Computation

- What is a neural network? An (arbitrary) directed acyclic graph (DAG)
- Forward computation: how you "use" a trained neural network.
  - Topological sweep (breadth-first)
  - Logistic regression  $\rho_{\theta}(y=1|x) = \sigma(w^{\top}x+b) = \frac{1}{1+\exp(-w^{\top}x-b)}$



### DAG ↔ Hypothesis Set

- What is a neural network? An (arbitrary) directed acyclic graph (DAG)
- Implication in practice
  - Naturally supports high-level abstraction
  - Object-oriented paradigm fits well.\*
    - Base classes: variable (input/output) node, operation node
    - Define the internal various types of variables and operations by inheritance
  - Maximal code reusability
    - See the success of PyTorch, TensorFlow, DyNet, ...
- You define a hypothesis set by designing a directed acyclic graph.
- The hypothesis space is then a set of all possible parameter settings.

### Supervised Learning

- Three points to consider both in research and in practice
  - 1. How do we decide/design a hypothesis set?
  - 2. How do we decide a **loss function**?
  - 3. How do we **optimize** the loss function?

#### Loss Functions

- Per-example loss function
  - Computes how good a model is doing on a given example:  $l(M(x),y) \ge 0$
- So many loss functions...
  - Classification: hinge loss, log-loss, ...
  - Regression: mean squared error, mean absolute error, robust loss, ...
- In this lecture, we stick to distribution-based loss functions.

# A Neural network computes a conditional distribution

• Supervised learning: what is y given  $x \ge 1$ 

$$f_{\theta}(x) = ?$$

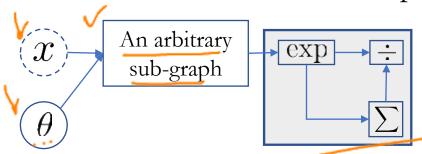
• In other words, how probable is a certain value y' of y given x?

$$p(y = y'|x) = ?$$

- What kind of distributions?
  - Binary classification: Bernoulli distribution
  - Multiclass classification: Categorical distribution
  - Linear regression: Gaussian distribution
  - Multimodal linear regression: Mixture of Gaussians

#### Important distributions – Categorical

- How probable is a certain value y' of y given x? p(y = y'(x) = ?
- Multi-class classification: Categorical distribution  $\mathcal{C}(\{\mu_1, \mu_2, \dots, \mu_C\})$ 
  - Probability:  $p(y = v | x) = \mu_v$ , where  $\sum \mu_v = 1$
  - Fully characterized by  $\{\mu_1, \mu_2, \dots, \mu_C\}^{v=1}$
  - A neural network then should turn the input x into a vector  $\mu =$



using a **softmax** function; softmax $(a) = \frac{1}{\sum_{v=1}^{C} \exp(a_v)} \exp(a)$ .

#### Important distributions – Gaussian

- How probable is a certain value y' of y given x? p(y = y'|x) = ?
- Regression: Gaussian distribution  $\mathcal{N}(\mu, \mathbb{I})$  with an identity covariance Probability:  $p(y|x) = \frac{1}{Z} \exp(-\frac{1}{2}(y-\mu)^{\top}(y-\mu))$ 

  - Fully characterized by  $\mu \in \mathbb{R}^q$ .
  - A neural network then should turn the input x into a vector  $\mu$ .
  - Can be done trivially by affine transformation.

### Loss Function – negative log-probability

- Once a neural network outputs a conditional distribution  $p_{\theta}(y|x)$  a natural way to define a loss function arises.
- Make sure training data is maximally likely:
  - Equiv. to making sure each and every training example is maximally likely.

$$\arg\max_{\theta} \log p_{\theta}(D) = \arg\max_{\theta} \sum_{n=1}^{N} \log p_{\theta}(y_n|x_n)$$

- Why log? many reasons... but out of the lecture's scope.
- Equivalently, we want to minimize the negative log-probability.
  - A loss function is the sum of negative log-probabilities of correct answers.

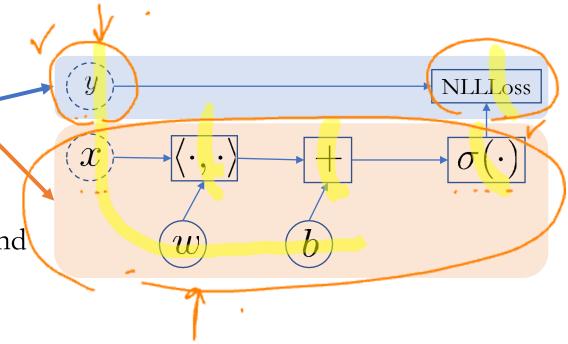
$$L(\theta) = \sum_{n=1}^{N} l(M_{\theta}(x_n), y_n) = \sum_{n=1}^{N} \log p_{\theta}(y_n(x_n))$$

### Loss Function – negative log-probability

- Once a neural network outputs a conditional distribution  $p_{\theta}(y|x)$ , a natural way to define a loss function arises.
- Practical implications
  - An OP node: negative log-probability (e.g., NLLLoss in PyTorch)
    - Inputs: the conditional distribution and the correct output
    - Output: the negative log-probability (a scalar)

### Loss Function – negative log-probability

- Once a neural network outputs a conditional distribution  $p_{\theta}(y|x)$ , a natural way to define a loss function arises.
- Logistic regression
  - Computes a Bernoulli distribution
  - Computes a negative log-probability.
  - All in one directed acyclic graph
- Forward computation
  - Computes the conditional distribution, and
  - Computes the per-example loss



### Supervised Learning

- Three points to consider both in research and in practice
  - 1. How do we decide/design a hypothesis set?
  - 2. How do we decide a loss function?
  - 3. How do we **optimize** the loss function?

#### Loss Minimization

- What we now know
  - 1. How to build a neural network with an arbitrary architecture.
  - 2. How to define a per-example loss as a negative log-probability.
  - 3. Define a single directed acyclic graph containing both.
- What we now need to know
  - 1. Choose an optimization algorithm.
  - 2. How to use the optimization algorithm to estimate parameters  $\theta$ .

#### Gradient-based optimization

- A continuous, differentiable\* function  $L(\mathbb{R}^d)$
- Given the current value  $\theta_0$ , how should I move to minimize L?
- Gradient descent

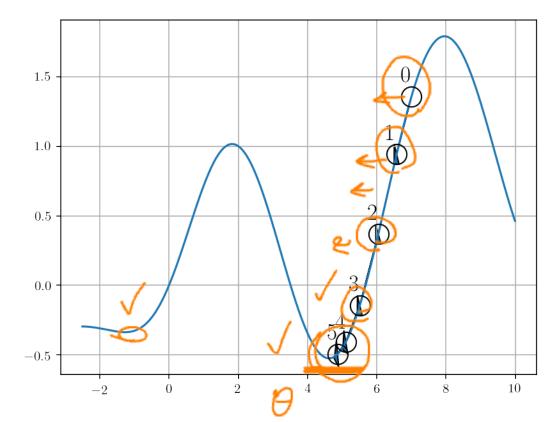
- ンレンシ
- The negative gradient of the function:  $-\nabla L(\theta_0)$
- This is only valid in a local neighbourhood of  $\theta_0$  take a very small step!

$$\theta = \theta_0 - \eta \nabla L(\theta_0)$$

- Efficient and effective even in the high dimensional space.
  - Can be improved with the second-order information (Hessian and/or FIM)

#### Gradient-based optimization

- A continuous, differentiable function  $L: \mathbb{R}^d \to \mathbb{R}$
- Given the current value  $\theta_0$ , how should I move to minimize L?
- Gradient descent
  - Efficient and effective even in the high dimensional space.
  - Learning rate must be carefully selected and annealed over time.



## Backward Computation - Backpropagation

- How do we compute the gradient of the loss function?
- 1. Manual derivation
  - Relatively doable when the DAG is small and simple.
  - When the DAG is larger and complicated, too much hassle.
- 2. Automatic differentiation (autograd)
  - Use the chain rule of derivatives

$$\frac{\partial (f) \circ (g)}{\partial (x)} = \frac{\partial (f)}{\partial (g)} \frac{\partial (g)}{\partial (x)} \qquad (x) \qquad (g)$$

- The DAG is nothing but a composition of (mostly) differentiable functions.
- Automatically apply the chain rule of derivatives.

### Backward Computation - Backpropagation

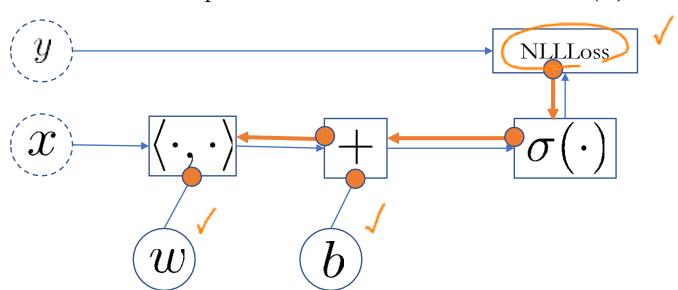
- Automatic differentiation (autograd)
  - 1. Implement the Jacobian-vector product of each OP node:

$$\begin{bmatrix} \frac{\partial L}{\partial x_1} \\ \vdots \\ \frac{\partial L}{\partial x_d} \end{bmatrix} = \begin{bmatrix} \frac{\partial F_1}{\partial x_1} & \cdots & \frac{\partial F_{d'}}{\partial x_1} \\ \vdots & \ddots & \vdots \\ \frac{\partial F_1}{\partial x_d} & \cdots & \frac{\partial F_{d'}}{\partial x_d} \end{bmatrix} \begin{bmatrix} \frac{\partial L}{\partial F_1} \\ \vdots \\ \frac{\partial L}{\partial F_{d'}} \end{bmatrix}$$

- Can be implemented efficiently without explicitly computing the Jacobian.
- The same implementation can be reused every time the OP node is called.

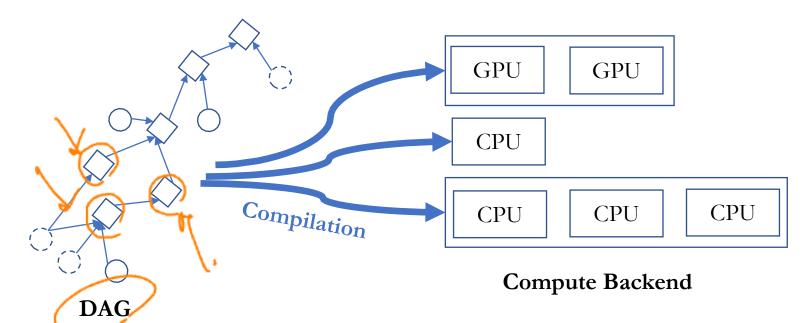
### Backward Computation – Backpropagation

- Automatic differentiation (autograd)
  - 2. Reverse-sweep the DAG starting from the loss function node.
    - Iteratively multiplies the Jacobian of each OP node until the leaf nodes of the parameters.
    - As expensive as forward computation with a constant overhead: O(N), where N: # of nodes.



#### Backward Computation – Backpropagation

- Practical Implications Automatic differentiation (autograd)
  - Unless a complete new OP is introduced, no need to manually derive the gradient
  - Nice de-coupling of specification (front-end) and implementation (back-end)
    - 1. [Front-end] Design a neural network by creating a DAG.
    - 2. [Back-end] The DAG is "compiled" into an efficient code for a target compute device.



#### Gradient-based Optimization

- Backpropagation gives us the gradient of the loss function w.r.t.  $\theta$
- Readily used by off-the-shelf gradient-based optimizers
  - Gradient descent, L-BFGS, Conjugate gradient, ...
  - Though, most are not applicable in a realistic neural network with 10s or 100s of millions of parameters.
- Stochastic gradient descent
  - Approximate the full loss function (the sum of per-examples losses) using only a small random subset of training examples:

$$\nabla L \approx \frac{1}{N'} \sum_{n=1}^{N'} \nabla l(M(x_{n'}), y_{n'}) \qquad \min_{m, n \in \mathcal{M}} \frac{1}{m'} \sum_{n=1}^{N'} \nabla l(M(x_{n'}), y_{n'})$$

#### Stochastic Gradient Descent

- Stochastic gradient descent
  - Approximate the full loss function (the sum of per-examples losses) using only a small random subset of training examples:

$$\nabla L \approx \frac{1}{N'} \sum_{n=1}^{N'} \nabla l(M(x_{n'}), y_{n'})$$

- Unbiased estimate of the full gradient.\*
- Learning rate must be annealed appropriately.
- Extremely efficient de facto standard practice.

#### Stochastic Gradient Descent

- Stochastic gradient descent in practice
  - 1. Grab a random subset of M training examples\*  $D' = \{(x_1, y_1), \dots, (x_{N'}, y_{N'})\}$
  - 2. Compute the minibatch gradient

$$\nabla L \approx \frac{1}{N'} \sum_{n=1}^{N'} \nabla l(M(x_{n'}), y_{n'})$$

- 3. Update the parameters  $\theta \leftarrow \theta + \eta \nabla L(\theta; D')$
- 4. Repeat until the validation loss stops improving.

\* In practice, sample without replacement until the training set is exhausted (one epoch).

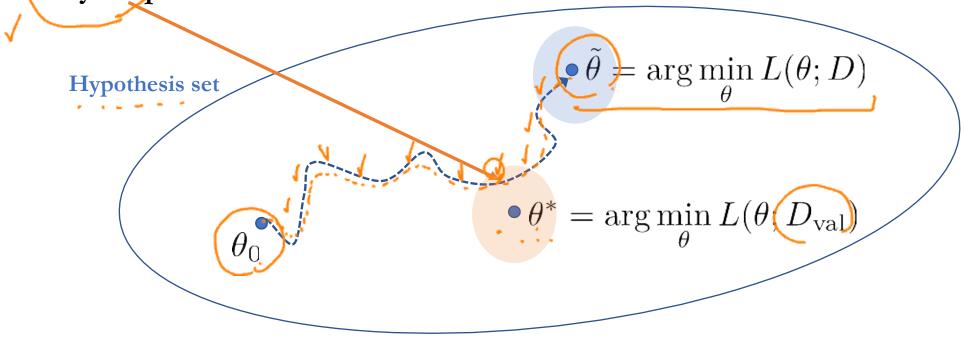
This is called early-stopping which prevents the neural network from overfitting to training examples.

### Stochastic Gradient Descent – Early Stopping

- Stochastic gradient descent in practice
  - 1. Grab a random subset of M training examples
  - 2. Compute the minibatch gradient
  - 3. Update the parameters
  - 4. Repeat until the validation loss stops improving.
- An efficient way to prevent overfitting
  - Overfitting: the training loss is low, but the validation loss is not.
  - The most serious problem in statistical machine learning.
  - Early-stop based on the validation loss

# Stochastic Gradient Descent – Early Stopping

- An efficient way to prevent overfitting
  - Overfitting: the training loss is low, but the validation loss is not.
  - The most serious problem in statistical machine learning.
  - Early-stop based on the validation loss



### Stochastic Gradient Descent

### Adaptive Learning Rate

- Stochastic gradient descent in practice
  - 1. Grab a random subset of M training examples  $D' = \{(x_1, y_1), \dots, (x_{N'}, y_{N'})\}$
  - 2. Compute the minibatch gradient
  - 3. Update the per-parameter learning rate  $\eta_{\theta}$
  - 4. Update the parameters

$$\theta \leftarrow \theta - \eta_{\theta} \frac{\partial L'}{\partial \theta}$$

- 5. Repeat until the validation loss stops improving.
- Adaptive learning rate: Adam [Kingma&Ba, 2015], Adadelta [Zeiler, 2015], and many more...
  - Approximately re-scale parameters to improve the conditioning of the Hessian.

### Supervised Learning with Neural Networks

- 1. How do we decide/design a hypothesis set?
  - Design a network architecture as a directed acyclic graph
- 2. How do we decide a **loss function**?
  - Frame the problem as a conditional distribution modelling
  - The per-example loss function is a negative log-probability of a correct answer
- 3. How do we **optimize** the loss function?
  - Automatic backpropagation: no manual gradient derivation
  - Stochastic gradient descent with early stopping [and adaptive learning rate]

# Language modeling as supervised learning

On the boundary between unsupervised and supervised learning

## Language Modelling

- Input: a sentence purpl ~
- Output: the probability of the input sentence
- A language model captures the distribution over all possible sentences.  $p(X) = p((x_1, x_2, ..., x_T))$
- It is unsupervised learning.
  - We will however turn the problem into a sequence of supervised learning.

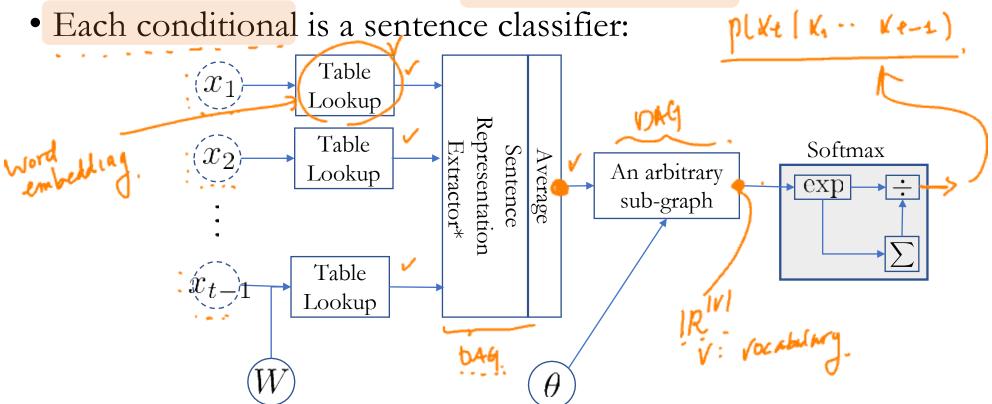
## Autoregressive language modelling

- Autoregressive sequence modelling
  - The distribution over the next token is based on all the previous tokens.  $p(X) = p(x_1)p(x_2|x_1) \cdots p(x_T|x_1, \dots, x_{T-1})$
  - This equality holds exactly due to the def. of conditional distribution.
- Unsupervised learning becomes a set of supervised problems.
  - Each conditional is a neural network classifier.
  - Input is all the previous tokens (a partial sentence).
  - Output is the distribution over all possible next tokens (classes).
  - It is a **text classification** problem.

## Autoregressive language modelling

- Autoregressive sequence modelling
  - The distribution over the next token is based on all the previous tokens.

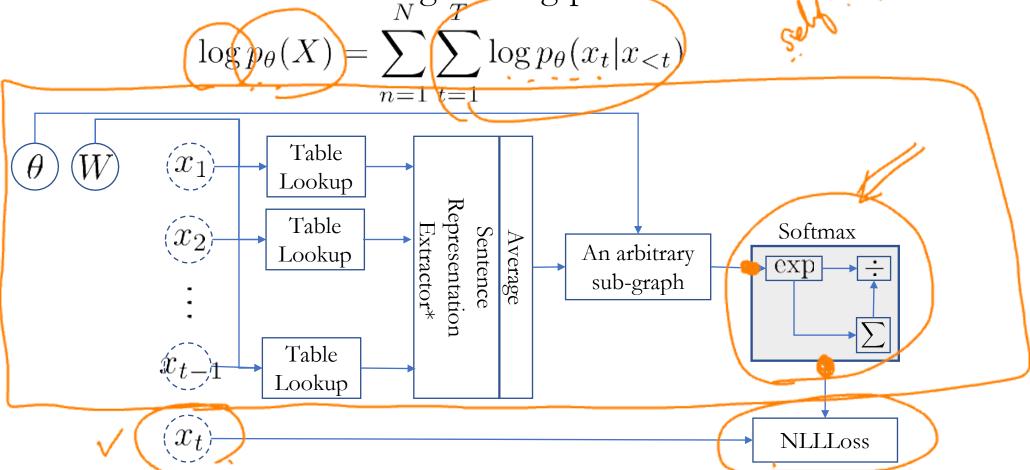
$$p(X) = p(x_1)p(x_2|x_1)\cdots p(x_T|x_1,\dots,x_{T-1})$$



## Autoregressive language modelling

• Autoregressive sequence modelling  $p(X) = \prod_{t=1}^{t} p(x_t | x_{< t})$ 

• Loss function: the sum of negative log probabilities



### Scoring a sentence

- Autoregressive sequence modelling
  - The distribution over the next token is based on all the previous tokens.

$$p(X) = p(x_1)p(x_2|\tilde{x}_1) \cdots p(x_T|\tilde{x}_1, \dots, \tilde{x}_{T-1}) \Leftrightarrow \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \mathbb{R}^d \mathbb{R}^d$$
natural way to score a sentence:

In Korea, more than half of residents speak Korean

- A natural way to score a sentence:
  - In Korea, more than half of residents speak Korean.
  - 'In' is a reasonable token to start a sentence.
  - "Korea" is pretty likely given "In"
  - "more" is okay token to follow "In Korea"
  - "than" is very likely after "In Korea, more"
  - "half" is also very likely after "In Korea, more than"

• Sum all these scores and get the sentence score.

### Scoring a sentence

- Autoregressive sequence modelling
  - The distribution over the next token is based on all the previous tokens.

$$p(X) = p(x_1)p(x_2|x_1)\cdots p(x_T|x_1,\ldots,x_{T-1})$$

- A natural way to score a sentence:
  - "In Korea, more than half of residents speak Korean." vs.

"In Korea, more than half of residents speak Finnish."

- The former is more likely (=higher probability) than the latter.
- This is precisely what NLLLoss computes over the sentence.

X1 ·· Xt-1 Xt Plyt X1·· Xt-1)

- Let's back up a little...
- What would we do without a neural network?
- Assume a Markovian property

$$p(X) = \prod_{t=1}^{T} p(x_t | x_{< t}) \approx \prod_{t=1}^{T} p(x_t | x_{t-n}, \dots, x_{t-1})$$

• This turned out to be crucial, and we will discuss why shortly.

$$p(X) = \prod_{t=1}^{T} p(x_t | x_{< t}) \approx \prod_{t=1}^{T} p(x_t | x_{t-n}, \dots, x_{t-1})$$

- We need to estimate *n*-gram probabilities:  $p(x)x_{-N}, x_{-N+1}, \dots, x_{-1}$

• Recall the def. of conditional and marginal probabilities: 
$$p(x|x_{-N},x_{-N+1},\ldots,x_{-1}) = \frac{p(x_{-N},x_{-N+1},\ldots,x_{-1},x)}{p(x_{-N},x_{-N+1},\ldots,x_{-1})} \text{ cmd. probabilities:}$$

$$= \frac{p(x_{-N},x_{-N+1},\ldots,x_{-1},x)}{\sum_{x \in V} p(x_{-N},x_{-N+1},\ldots,x_{-1},x)}$$

• V: all possible tokens (=vocabulary)

• We need to estimate *n*-gram probabilities:

$$p(x|x_{-N}, x_{-N+1}, \dots, x_{-1}) = \frac{p(x_{-N}, x_{-N+1}, \dots, x_{-1}, x)}{\sum_{x \in V} p(x_{-N}, x_{-N+1}, \dots, x_{-1}, x)}$$

- How do we estimate the probability?
  - I want to estimate the probability of my distorted coin landing head.
  - Maximum likelihood estimation (MLE): toss the coin a lot and look at how often it lands heads.

Data Collection

Estimation

• We need to estimate *n*-gram probabilities:

$$p(x|x_{-N}, x_{-N+1}, \dots, x_{-1}) = \frac{p(x_{-N}, x_{-N+1}, \dots, x_{-1}, x)}{p(x_{-N}, x_{-N+1}, \dots, x_{-1})}$$

- Data: all the documents or sentences you can collect
  - e.g., Wikipedia, news articles, tweets, ...
- Estimation:
  - 1. Count the # of occurrences for the *n*-gram  $(x_{-N}, x_{-N+1}, \dots, x_{-1}, x)$
  - 2. Count the #'s of occurrences for all the *n*-grams of the form:

$$(x_{-N}, x_{-N+1}, \dots, x_{-1}, ?)$$

• We need to estimate *n*-gram probabilities:

$$p(x|x_{-N}, x_{-N+1}, \dots, x_{-1}) = \frac{p(x_{-N}, x_{-N+1}, \dots, x_{-1}, x)}{p(x_{-N}, x_{-N+1}, \dots, x_{-1})}$$

• Estimation:

Estimation: 
$$p(x|x_{-N}, x_{-N+1}, \dots, x_{-1}) = \frac{p(x_{-N}, x_{-N+1}, \dots, x_{-1}, x)}{\sum_{x \in V} p(x_{-N}, x_{-N+1}, \dots, x_{-1}, x)}$$

$$\approx \frac{c(x_{-N}, x_{-N+1}, \dots, x_{-1}, x)}{\sum_{x \in V} c(x_{-N}, x_{-N+1}, \dots, x_{-1}, x')}$$

• Do you see why this makes sense?

count

• We need to estimate n-gram probabilities:

$$p(x|x_{-N}, x_{-N+1}, \dots, x_{-1}) = \frac{p(x_{-N}, x_{-N+1}, \dots, x_{-1}, x)}{\sum_{x \in V} p(x_{-N}, x_{-N+1}, \dots, x_{-1}, x)}$$

$$\approx \frac{c(x_{-N}, x_{-N+1}, \dots, x_{-1}, x)}{\sum_{x' \in V} c(x_{-N}, x_{-N+1}, \dots, x_{-1}, x')}$$

• How likely is "University" given "New York"?



- Count all "New York University"
- Count all "New York?": e.g., "New York State", "New York City", "New York Fire", "New York Police", "New York Bridges", ...
- How often "New York University" happens among these?

# NGram Language Models – Two problems

- Data sparsity: lack of generalization
  - What happens "one" n-gram never happens?  $p(a \text{ lion is chasing a llama}) \neq p(x) \times p(\text{lion}|a) \times p(\text{is lion})$



 $p(\text{chasing}|\text{kon is}) \times p(\text{a}|\text{is} \text{chasing})$ 

 $\times p(\text{llama}|\text{chasing a})$ 

- Inability to capture long-term dependencies
  - Each conditional only considers a small window of size *n*.
  - Consider "the same stump hich had impaled the car of many a guest in the past thirty years and which he refused to have removed
  - It is impossible to tell "removed" is likely by looking at the four preceding tokens.

### Traditional Solutions

#### Data Sparsity

• Smoothing: add a small constant to avoid 0.

$$p(x|x_{-N}, x_{-N+1}, \dots, x_{-1}) \approx \frac{c(x_{-N}, x_{-N+1}, \dots, x_{-1}, x) + \epsilon}{\epsilon |V| + \sum_{x' \in V} c(x_{-N}, x_{-N+1}, \dots, x_{-1}, x')}$$

• Backoff: try a shorter window. 
$$c(x_{-N},\ldots,x) = \begin{cases} c(x_{-N+1},\ldots,x) + \beta, & \text{if } c(x_{-N},\ldots,x) = 0 \\ c(x_{-N},\ldots,x), & \text{otherwise} \end{cases}$$

- The most widely used approach: Kneser-Ney smoothing/backoff
- KenLM implements the efficient n-gram LM model.

### Traditional Solutions

#### 2. Long-Term Dependency

- Increase *n*: not feasible as the data sparsity worsens.
- # of all possible *n*-grams grows exponentially w.r.t. *n*:  $O(|V|^n)$
- The data size does not grow exponentially: many never-occurring *n*-grams.
- These two problems are closely related and cannot be tackled well.
  - To capture long-term dependencies, *n* must be large.
  - To address data sparsity, *n* must be small.
  - Conflicting goals..

Count-based

### N-Gram Language Models – Two problems

- 1. Data sparsity: lack of generalization
  - What happens "one" n-gram never happens?

$$p(a \text{ lion is chasing a llama}) = p(a) \times p(\text{lion}|a) \times p(\text{is}|a \text{ lion})$$

$$\times p(\text{chasing}|\text{lion is}) \times p(\text{a}|\text{is chasing})$$

$$\times p(\text{llama}|\text{chasing a}) = 0$$

=0

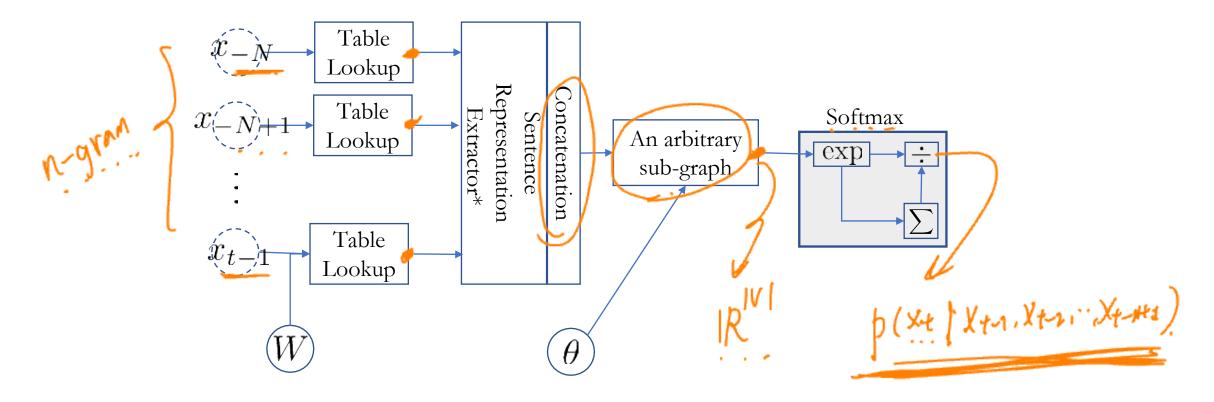
- 2. Inability to capture long-term dependencies
  - Each conditional only considers a small window of size *n*.
  - Consider "the same **stump** which had impaled the car of many a guest in the past thirty years and which he refused to have **removed**
  - It is impossible to tell "removed" is likely by looking at the four preceding tokens.

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### Freed forward

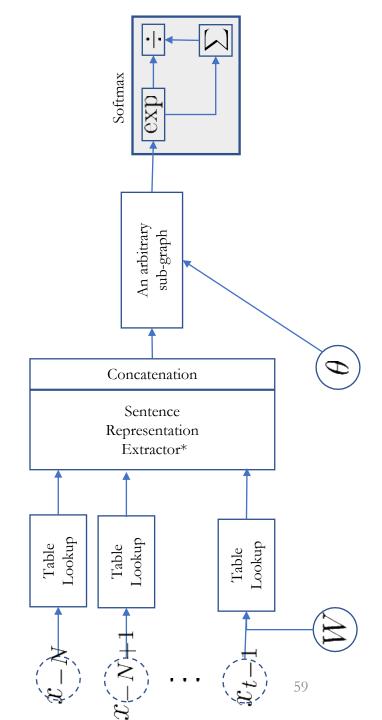
### Neural N-Gram Language Model [Bengio et al., 2001]

• The first extension of n-gram language models using a neural network

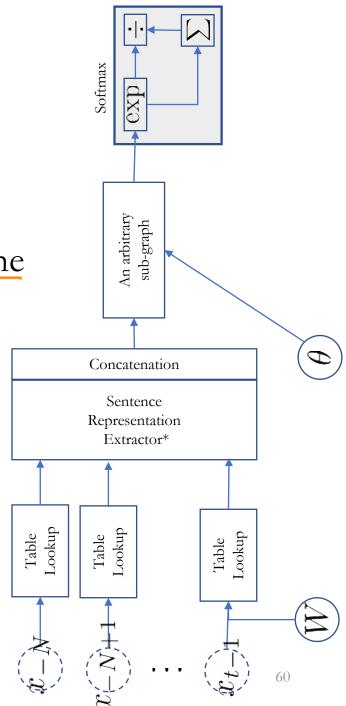


- The first neural language models
- Trained using backpropagation and SGD
- Generalizes to an unseen *n*-gram
- Addresses the issue of data sparsity

• *How?* 

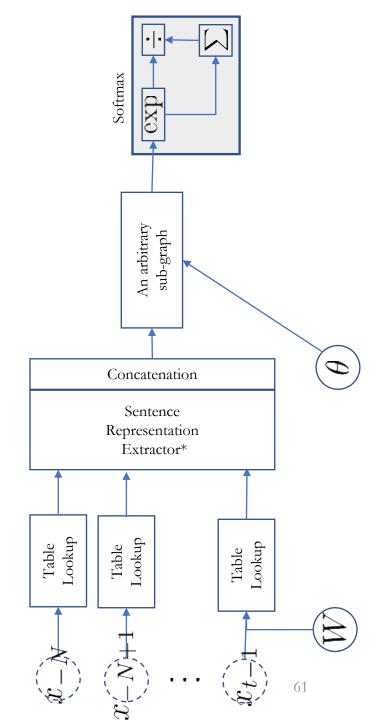


- Why does the data sparsity happen?
- A "shallow" answer: some n-grams do not occur in the training data, while they do in the test time.
- A "slightly deeper" answer: it is difficult to impose token/phrase similarities in the discrete space.



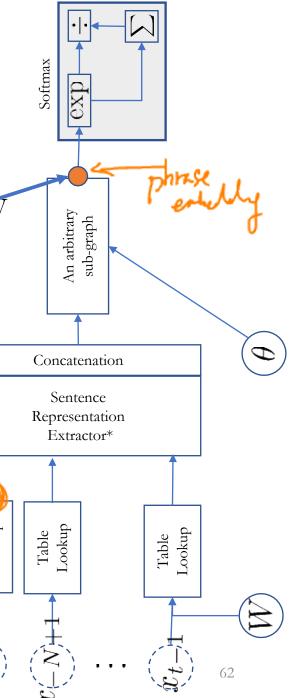
- Why does the data sparsity happen?
- Back to the earlier example
  - Problem:  $c(\text{chasing a llama}) = 0 \ \, \checkmark$ .
  - Observation:  $c(\text{chasing a cat}) \gg 0$   $c(\text{chasing a dog}) \gg 0$   $c(\text{chasing a deer}) \gg 0$

• If the LM knew "llama" is a mammal similar to "cat", "dog" and "deer", it would be able to guess "chasing a llama" is as likely as "chasing a cat", "chasing a dog", and "chasing a deer".



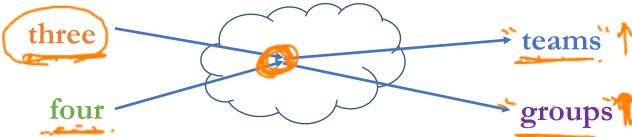
- The neural n-gram language model addresses this issue by "learning the similarities" among tokens and phrases in a "continuous vector space".
- In the "continuous vector space", similar tokens/phrases are nearby: e.g., word2vec [Mikolov et al., 2013; Pennington et al., 2014], doc2vec [Le&Mikolove, 2014], sentence-to-vec [Hill et al., 2016 and ref's therein]
- Then, similar input n-grams lead to similar output:

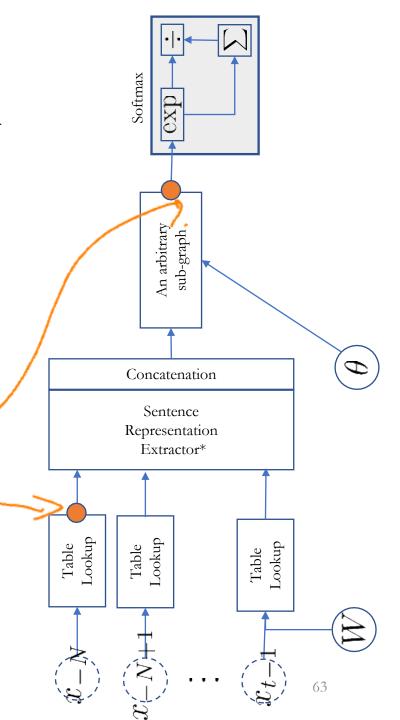
$$D(x_t|x_{t-N},\ldots,x_{t-1}||x_t|x'_{t-N},\ldots,x'_{t-1}) < \epsilon$$



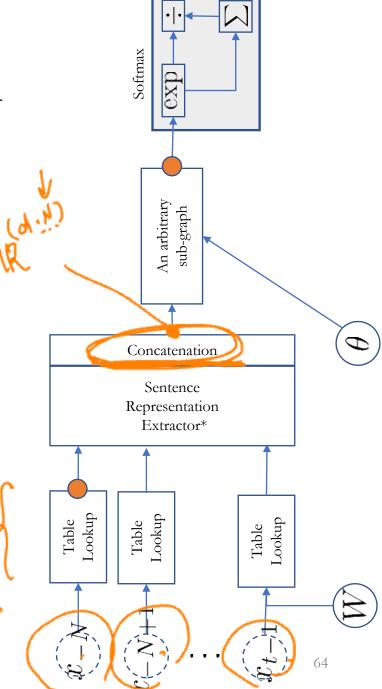
- Training examples
  - there are three teams left for qualification.
  - four teams have passed the first round.
  - four groups are playing in the field.
- Q: how likely is "groups" followed by "three"?

Continuous vector space





- In practice,
- 1. Collect all n grams from the corpus
- 2. Shuffle all the n-grams to build a training set
- 3. Train the neural n-gram language model using stochastic gradient descent on minibatches containing 100-1000 n-grams.
- 4. Early-stop based on the validation set.
- 5. Report perplexity on the test set.  $ppl = b^{\frac{1}{|D|} \sum_{(x_1, ..., x_N) \in D} \log_b p(x_N | x_1, ..., x_{N-1})}$



### Infinite context $n \rightarrow \infty$

## - CBoW Language Models

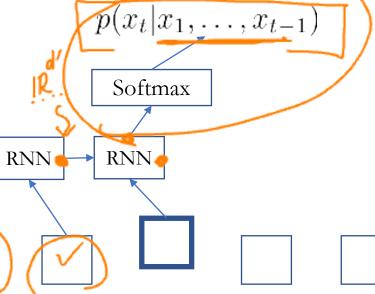
- Equivalent to the neural LM after replacing "concat" with "average"
  - "Averaging" allows the model to consider the infinite large context window.
- Extremely efficient, but a weak language model
  - Ignores the order of the tokens in the context windows.
    - Any language with a fixed order cannot be modelled well.
  - Averaging ignores the absolute counts, which may be important:
    - If the context window is larger, "verb" becomes less likely in SVO languages.

### Infinite context $n \rightarrow \infty$

- Recurrent Language Models [Mikolov et al., 2010]
- A recurrent network summarizes all the tokens so far.
- Use the recurrent network's memory to predict the next token.

**RNN** 

- Efficient online processing of a streaming text:
  - Constant time per step.
  - Constant memory throughout forward computation.
- Useful in practice:
  - Useful for autocomplete and keyword suggestion.
  - Scoring partial hypotheses in generation.



### Infinite context $n \rightarrow \infty$

- Recurrent Memory Networks [Tran et al., 2016]

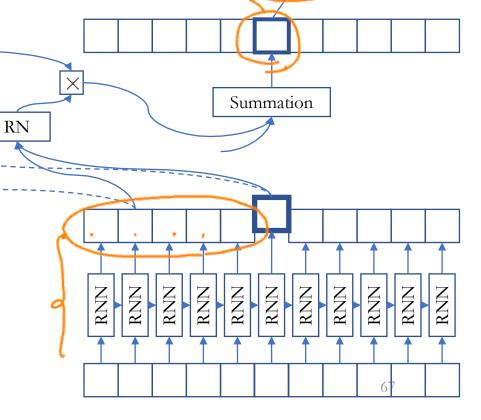
• The **recurrent network** solves a difficult problem: *compress the entire context into a fixed-size memory vector*.

• Self-attention does not require such compression but still can capture long-term dependencies.

Weighting Function  $\alpha$ 

• Combine these two: a recurrent memory network (RMN) [Tran et al., 2016]

• RNMT+: a similar, recent extension for neural machine translation



 $p(x_t|x_1,\ldots,x_{t-1})$ 

Softmax

### In this lecture, we learned

• What autoregressive language modelling is:

$$p(X) = p(x_1)p(x_2|x_1)\cdots p(x_T|x_1,\ldots,x_{T-1})$$

- How autoregressive language modelling transforms unsupervised learning • It is a series of predicting the next token given previous tokens.
- How neural language modelling improves upon n-gram language models:
  - Continuous vector space facilitates generalization to unseen n-grams.
  - Infinitely large context window
- How sentence representation extraction is used for language modelling:
  - Convolutional language models, recurrent language models and self-attention language models...